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## An Exploration of a Stochastic Model of Solute Transport

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# An Exploration of a Stochastic Model of Solute Transport

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## Background

A model of groundwater solute transport is being developed by Don Kulasiri (Kulasiri, 1997). This is part of a larger project being undertaken by Lincoln Environmental. In the model, the velocity of the water in the porous media has a component which is dependent on piezometric head according to Darcy's law, and a random component. The latter represents the variation which has been observed and which is assumed to be due to the porous media. The model also represents the diffusive process experienced by the solute in both a deterministic (Fick's law) and random manner. Thus we have a model which comprises stochastic partial differential equations in 3 dimensions.

The difficulty confronted by the model developer is how to get a good understanding of the behaviour of the model and thus have more confidence that it is working as expected. This short paper describes some attempts to visualise the behaviour of this model and shows how some inadequacies in its early implementation were discovered and a better understanding of the model's behaviour was obtained.

## The Model Details

The model equation which describes the velocity of fluid in the porous media is (Kulasiri, 1997):

$$\underline{V}(x, t) = \frac{d\underline{x}(t)}{dt} = -\frac{K(x)}{\varphi(x)} \nabla \phi(x, t) + \underline{W}(x, t) \quad (\text{Error! Bookmark not defined.1})$$

where

$\underline{V}(x, t)$  is the fluid velocity

$\underline{x}(t)$  is position in 3 dimensional space

$K(x)$  is hydraulic conductivity. Note that in general the medium may be anisotropic, in which case  $K$  would be a tensor. See Bear and Verruijt (1987, p 35) for details.

$\varphi(x)$  is porosity

$\phi(x, t)$  is piezometric head

$\underline{W}(x, t)$  is a stochastic (Wiener) component of velocity due to pore structure

Integration of equation (1) gives:

$$d\underline{x} = -\frac{K(\underline{x})}{\varphi(\underline{x})} \nabla \phi(\underline{x}, t) dt + d\underline{\beta}(t) \quad (2)$$

where

$d\underline{\beta}(\underline{x}, t) = \underline{W}(\underline{x}, t) dt$  is the increment due to the random component. It is calculated using

$$d\beta_q = e_q \sqrt{s_q} (N(0,1) + N(0,1)) \sqrt{dt} \quad (3)$$

where

$q$  represents the direction  $x$ ,  $y$  or  $z$

$N(0,1)$  is a standard normal variate. Note that two different Normal variate values are required.

$e_q$  is the eigenfunction in the direction  $q$  of the matrix which models the space correlation due to the Wiener process  $W$

$s_q$  is the magnitude of the stochastic Wiener velocity component in the direction  $q$

See Kulasiri (1997) for details of the calculation of  $d\underline{\beta}(t)$  and the numerical solution of the model equations.

The equation which describes the flux of solute is

$$\underline{J}(\underline{x}, t) = \underline{V}(\underline{x}, t) C(\underline{x}, t) - (D(\underline{x}) + R(\underline{x}, t)) \nabla C(\underline{x}, t) \quad (4)$$

where

$\underline{J}(\underline{x}, t)$  is the solute flux

$D(\underline{x})$  is the Fick diffusion coefficient

$C(\underline{x}, t)$  is the concentration of solute

$R(\underline{x}, t)$  is the random (Wiener) component of the diffusion

Note that the diffusive process is assumed to be isotropic. If this is not so,  $D$  and  $R$  will be tensors. See Bear and Verruijt (1987, p 159) for details.

The numerical solution of equation (4) is carried out as for equation (1) with the Wiener component being handled in a manner equivalent to equation (3). The relevant parameters are:

$\underline{u}_q$  the eigenfunction in the direction  $q$  of the matrix which models the space correlation of the Wiener process  $R$

$w_q$  the magnitude of the stochastic component of the Wiener process  $R$  in the direction  $q$ .

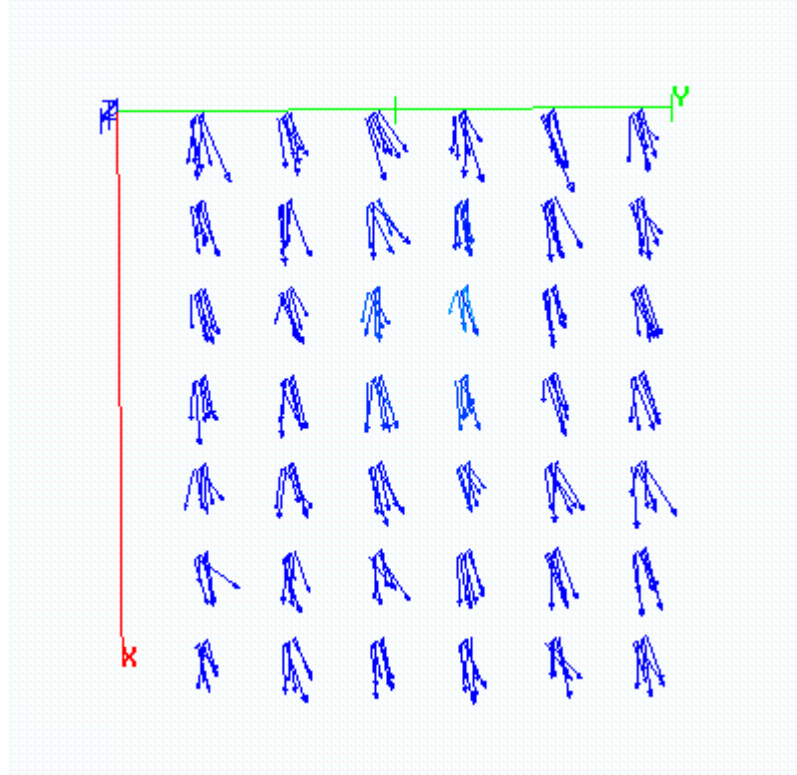
A numerical solution to the model equations as outlined above was programmed in C (Kulasiri, 1997). The base set of parameters shown in Table 1 was used for the simulations reported here unless otherwise stated. Where a parameter is listed as having a constant value, it is assumed not to vary with  $x$ . Unless otherwise stated the simulations were carried out over a  $20 \times 20 \times 20$  grid corresponding to a cube with 2.0m sides. A pulse of solute of concentration of  $0.25 \text{ g/m}^3$  was introduced along a vertical line in the  $x=0$  plane at position  $y=1.0\text{m}$  for a period of 0.1 days. Simulations were run for 0.5 days. The results of the simulations were written to a file at every 0.01 days and subsequently imported into AVS v5.0 (Advanced Visual Systems) for visualisation.

**Table 1** Base parameter values

Parameter	Units	Value
$K(x)$	$m/day$	46.0
$\phi(x)$		0.3
$e_x$		0.707
$e_y$		0.707
$e_z$		0.707
$dt$	$days$	0.001
$\nabla_x \phi$	$m \text{ of water}/m$	-0.002105
$\nabla_y \phi$	$m \text{ of water}/m$	0.0
$\nabla_z \phi$	$m \text{ of water}/m$	0.0
$s_x$	$m^2/day$	0.04
$s_y$	$m^2/day$	0.04
$s_z$	$m^2/day$	0.04
$D$	$m^2/day$	0.0000864
$u_x$		0.707
$u_y$		0.707
$u_z$		0.707
$w_x$	$m^4/day^3$	0.000002
$w_y$	$m^4/day^3$	0.000002
$w_z$	$m^4/day^3$	0.000002

### Fluid Velocity Calculation

While exploring the behaviour of the velocity equation, a number of results similar to that shown in Figure 1 were obtained. Here we see vectors displayed showing the magnitude and direction of the velocity.



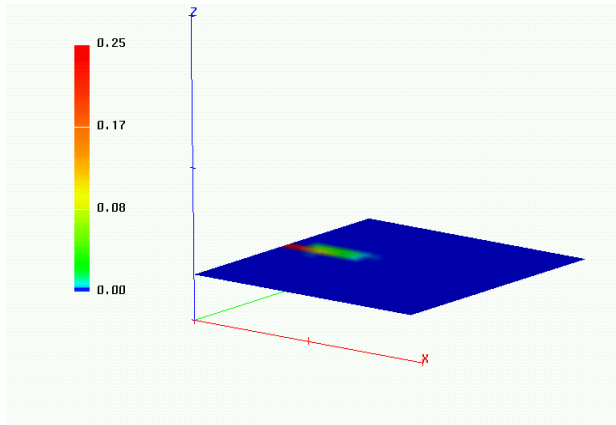
**Figure 1** A view of velocity vectors taken at 0.2 days. The view is looking down on the xy plane from the positive z direction. The length of each arrow is proportional to velocity magnitude. Note the tendency of the vectors to point in the positive y direction.

Given the base parameters, one would expect the velocity vectors to point in the positive x direction because of the piezometric head and to be evenly distributed in the positive and negative y directions due to the random component. It is apparent that they are biased in the positive y direction and were consistently so across a number of simulations. Subsequent testing of the random number generator programmed into the model showed it indeed had a bias. The algorithm used was published in Law and Kelton (1991, p454) although it was not determined whether the bias was due to a programming error or an error in the basic algorithm. This bias was removed by replacing the random number generator with one from Numerical Recipes (Press, 1992).

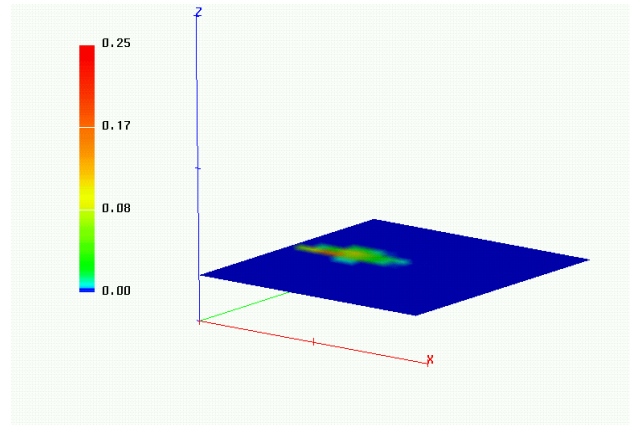
### Calculation of Solute Concentration

With the random number generator corrected we could proceed to explore the model's predictions of solute concentration.

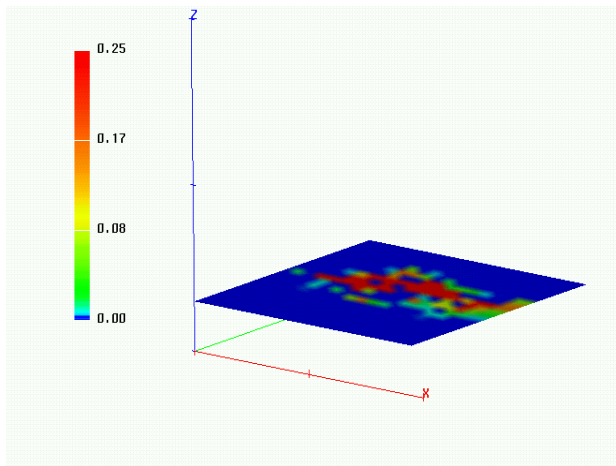
Figure 2 shows concentration values in an xy plane at  $z=0.3\text{m}$  taken at various times during the simulation.



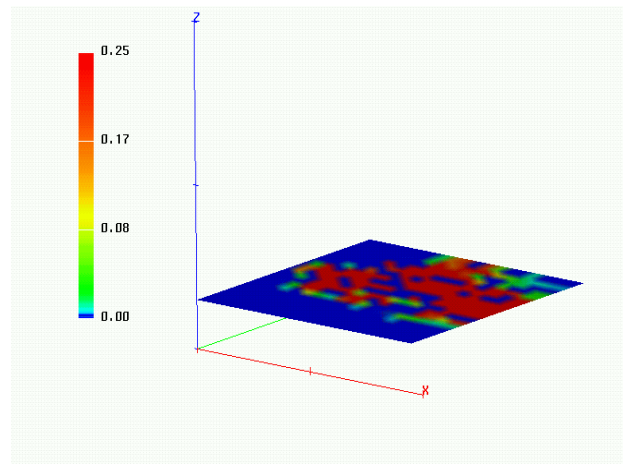
a) Concentration at 0.08 days



b) Concentration at 0.14 days



c) Concentration at 0.38 days



d) Concentration at 0.50 days

**Figure 2** Concentration of solute, indicated by colour, in the plane at  $z = 0.3$  m at various times following an input of solute along the line  $y = 1.0$  m in the  $x = 0$  plane for 0.1 days.

Note how the solute concentration in the frame at  $t = 0.08$  days (Figure 2a) is distributed as might be expected with the region of highest concentration being near the solute source at  $x = 0.0$  m,  $y = 1.0$  m.

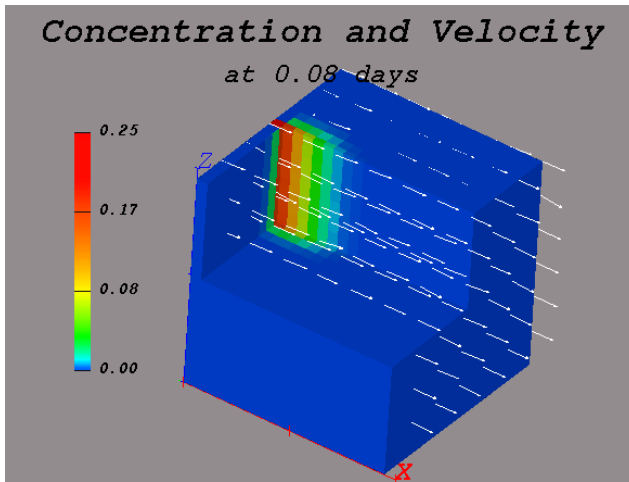
By  $t = 0.14$  days (Figure 2b) the solute source has been turned off and we see the solute has dispersed predominantly in the positive  $x$  direction with some lateral dispersion that might reasonably be expected, given the diffusive processes included in the model.

However, at 0.38 days (Figure 2c) and 0.50 days (Figure 2d) it is clear that there is some problem with the implementation of the model. At both these times the concentration has increased to its original value and perhaps higher and over a larger region than at 0.14

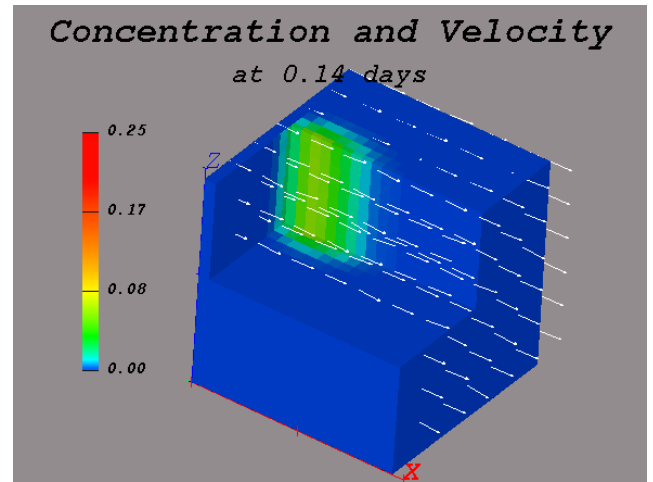
days. Clearly there is now more solute in the system than the amount which entered through the source at  $x = 0, y = 1.0$  m. Planes at different values of  $z$  showed similarly unsatisfactory concentrations.

This led to a review of the implementation of the model where errors were found in the calculations which determined the concentration increments throughout the 3D space at each time step.

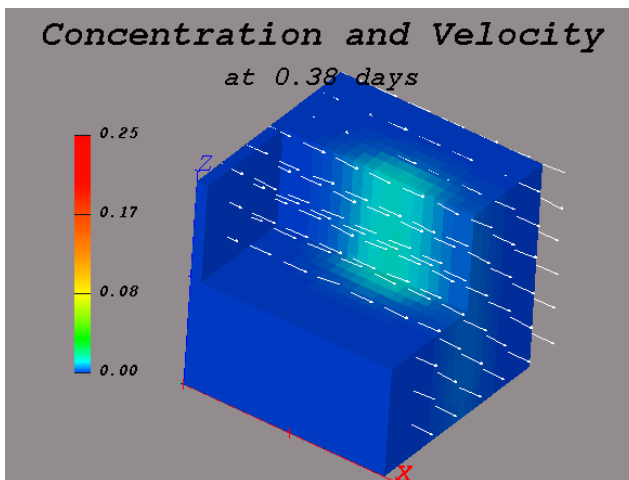
When these errors were corrected the solute distributions shown in Figure 3 were obtained. These conform to how one might expect such a system to behave.



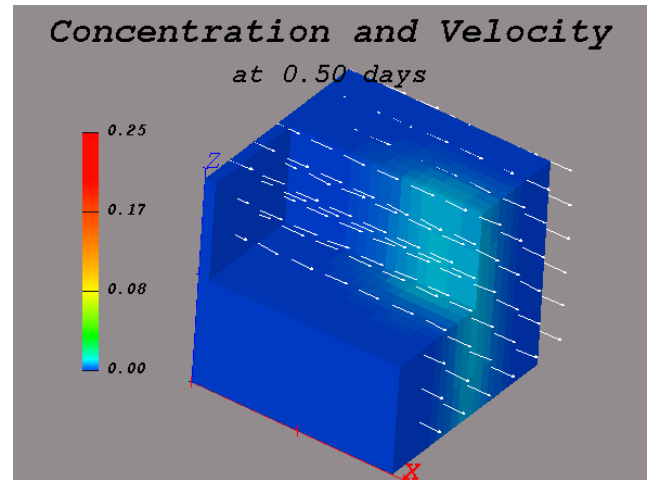
a) Concentration and Velocity at 0.08 days



b) Concentration and Velocity at 0.14 days



c) Concentration and Velocity at 0.38 days



d) Concentration and Velocity at 0.50 days

**Figure 3** Solute concentrations and velocity vectors following correction of model implementation errors apparent in Figure 2.



## **Aggregate behaviour of the velocity equation**

The simulation results shown in Figures 1-3 all result from single runs of the model although a large number of runs were actually carried out to ensure that those shown are representative of model behaviour. However, to get a better understanding of the influence of the random components of the model there is a need to aggregate model behaviour over a number of runs. This section reports a method developed for doing this for the velocity equation.

Integration of the model's velocity equation gives the trajectory in 3 dimensional space that would be traced by a weightless tracer particle if it were introduced into the field at some initial point. As pointed out above, this would give just one of a large number of possible trajectories so some aggregation is required.

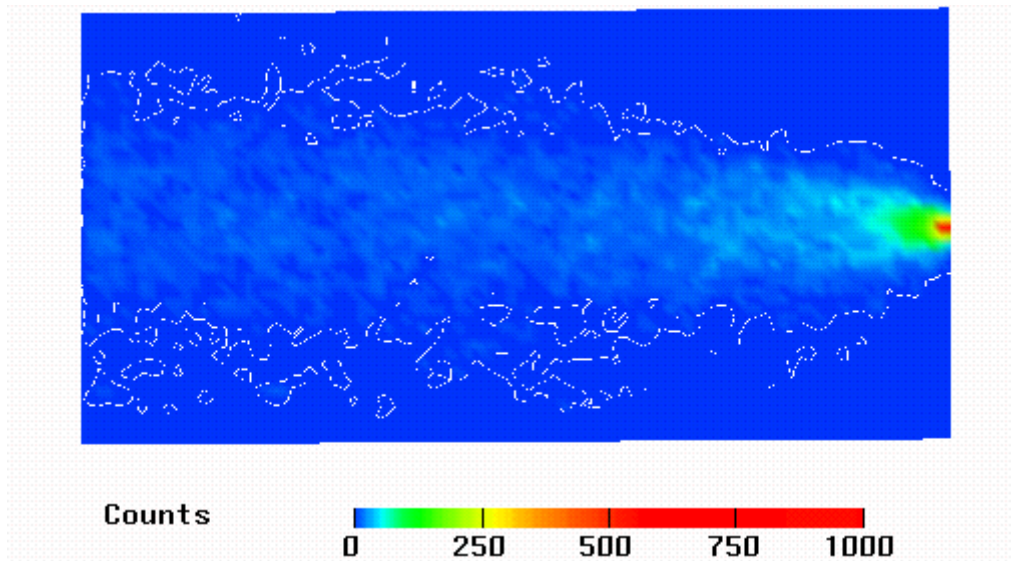
The approach taken is to determine the number of times each point on a 3 dimensional grid throughout the volume of interest is passed through by such a trajectory. This count, when taken over a sufficiently large number of trajectories, gives a type of 3 dimensional frequency distribution describing the behaviour of the stochastic and deterministic components in the model.

To achieve this, relevant parts of the original program were included in a new program which repeatedly integrated the velocity equation on a grid of 100x50x50 points in x, y, and z respectively with an interval of 0.1m between points. The initial point for each trajectory was position (0,2.5,2.5)m.

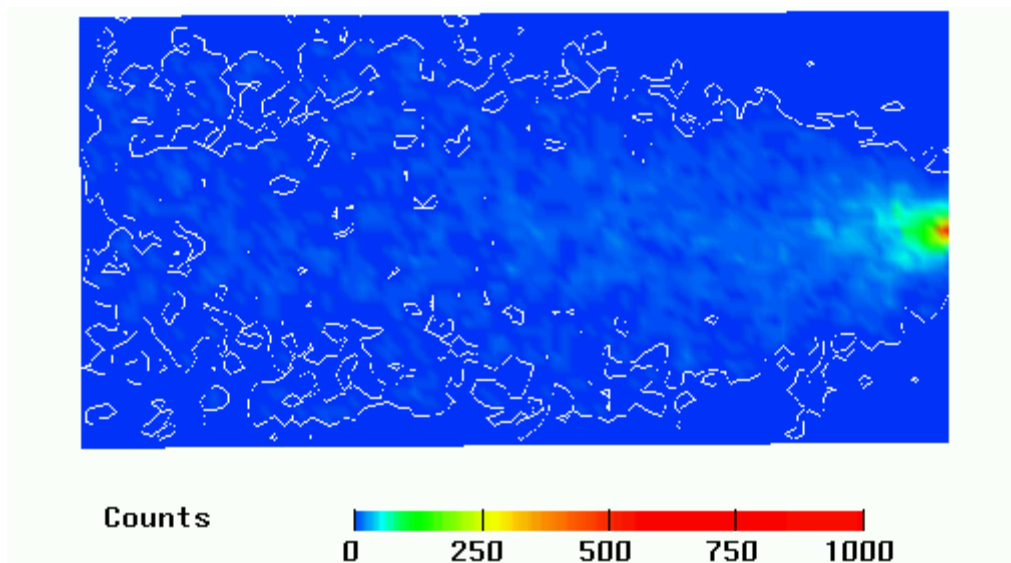
Because there is no reason for a trajectory to pass through a given grid point exactly, a calculation was done at each integration step to determine which grid point was the closest to the trajectory's current position. The trajectory was considered to have passed through that closest point and the point's visit count was incremented accordingly.

The solution for a particular trajectory terminated when the trajectory went outside the bounds of the 3 dimensional grid. 1000 trajectories were calculated for each set of parameters.

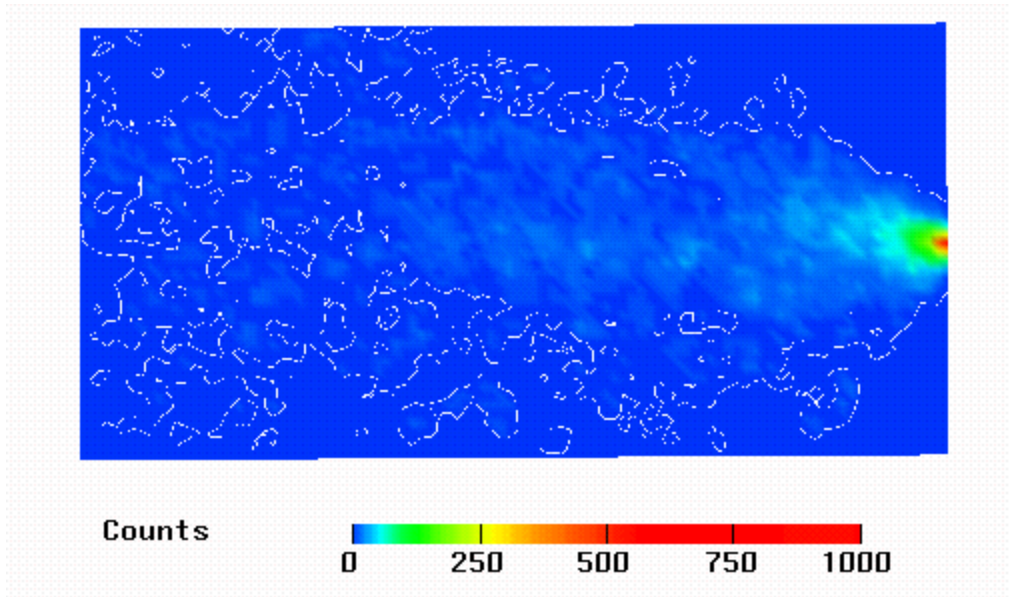
The results of 4 runs are shown in figures 4-7. The figure captions indicate how the parameters were varied from their base values. Each figure shows a normalised colour map of the number of counts on an x-z plane taken at a y value of 2.5m. Because every trajectory starts at the point (0,2.5,2.5)m and the parameters have the same values in the y and z directions, the counts will be circularly symmetric about the initial point so long as the number of trajectories is sufficiently large.



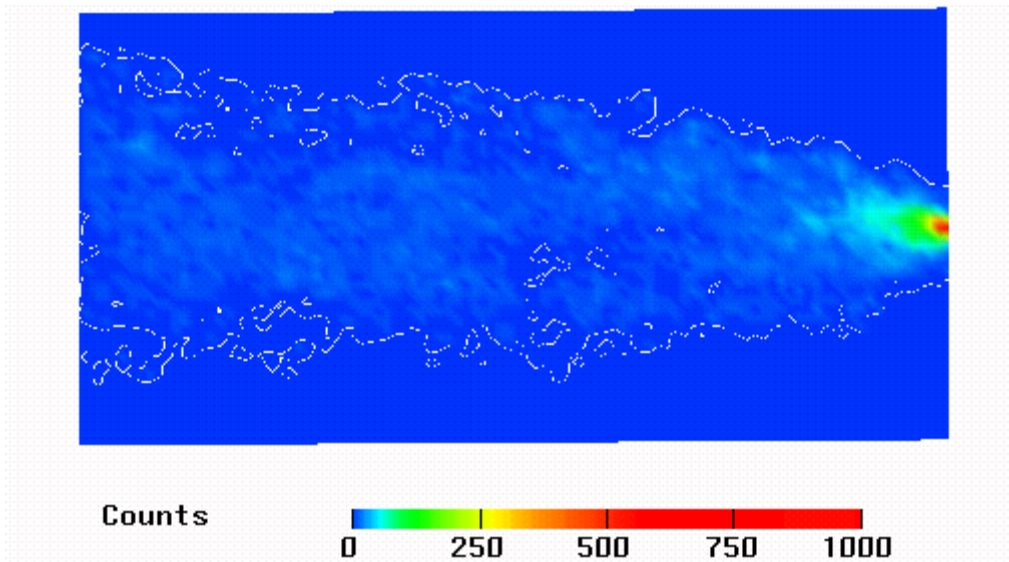
**Figure 4** Colour map of normalised trajectory visit counts for the base parameter set with  $dt=0.01$ . The white lines trace a boundary where the normalised counts are 1.  $X=0$  is at the right of the figure with the positive  $x$  direction being towards the left.



**Figure 5** Colour map of trajectory visit counts with  $s_x=s_y=s_z=0.1$  and  $dt=0.01$ . The white lines trace a boundary where the normalised counts are 1.  $X=0$  is at the right of the figure with the positive  $x$  direction being towards the left.



**Figure 6** Colour map of trajectory visit counts with  $\nabla_x \phi = -0.00105$  and  $dt=0.01$  The white lines trace a boundary where the normalised counts are 1.  $X=0$  is at the right of the figure with the positive  $x$  direction being towards the left.



**Figure 7** Colour map of trajectory visit counts with  $dt=0.001$  The white lines trace a boundary where the normalised counts are 1.  $X=0$  is at the right of the figure with the positive  $x$  direction being towards the left.

## Discussion

The work shown here demonstrates how even fairly basic use of a scientific visualisation systems such as AVS can help in the exploration of a model. In this case a number of issues related to the early implementation of a model of ground water solute dispersion were explored and corrected and a scheme was developed to give an aggregate view of the random behaviour of the model's velocity equation.

The aggregate views of the behaviour of the velocity equation shown in figures 4-7 are in reasonable accord with what one might expect. The counts near the initial point are high as would be expected as every trajectory needs to pass through this region although some will terminate quickly by passing through the  $x=0$  boundary. The extent to which that happens depends on the relative size of the deterministic flow in the positive  $x$  direction due to the piezometric head and the Wiener component, which may be negative, in the same direction. The count distribution is broader in cases where either the lateral Wiener components are increased in value as in Figure 5 or the piezometric head is decreased in value giving more opportunity for lateral dispersion to occur as in Figure 6.

The shape of the distribution in Figure 7 compared to that in Figure 4 is similar, although the normalised boundaries are a little narrower in Figure 7 especially in the region away from the initial point. This point needs further investigation as any sensitivity to  $dt$  is undesirable.

There is no claim here that visualisation tools obviate the need for careful programming and rigorous review of the numerical procedures involved in modelling and simulation. Nevertheless, the visualisation tools do allow the model's behaviour to be explored and criticised by people who have a conceptual understanding of how a system operates but do not have the time and/or expertise to comment on its complex mathematical and computational representations.

## Future Work

The work reported here comprises some useful, but elementary visualisations of what is a very complex model. One of the most interesting facets of the model is its inherently random nature. The work with the velocity equation reported here is an attempt to give an aggregate view of model behaviour for that case, but further work needs to be done to develop a scheme for aggregate viewing of overall model behaviour.

In addition to that, schemes need to be developed to increase the number of variables whose values are displayed throughout the 3D volume. As parameters such as conductivity are given a spatial variation, it is highly desirable to have the solute concentration being visualised against a background showing the conductivity variation.

## Acknowledgements

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